DRAFT

# Appendix K
# Interpolation Methods for Delineating Areas with RAL Exceedances

# 1 Overview of Data Interpolation Approach

This appendix presents the data interpolation method selection, application, and results to delineate the remedial action level (RAL) exceedance areas in the upper reach of the Lower Duwamish Waterway (LDW), as well as an uncertainty analysis to assess the level of confidence in the RAL exceedance area boundaries.

Interpolation methods use a local neighborhood of surrounding data points to estimate values (e.g., concentrations, probabilities of exceedance, or other physical or chemical parameters) at all unsampled points in the project area. Interpolation methods are commonly used to support remedial design (RD) and delineate areas requiring remedial action at sediment cleanup sites (e.g., Thornburg et al. 2005; Anchor QEA 2014; Anchor QEA and Tetra Tech 2016; City of Tacoma 2002).

The interpolation method and its application in the upper reach were developed in coordination with the US Environmental Protection Agency (EPA) interpolation technical team, including meetings on September 22; October 6, 14, 19, 20, and 27; November 9 and 16; and December 14, 2021. The interpolation work group consisted of EPA and its consultants (Syracuse Research Corporation [SRC] and HTSC) and the Lower Duwamish Waterway Group (LDWG) and its consultants (Anchor QEA and Windward Environmental LLC).

An overview of the upper reach interpolation approach is presented in the flow chart in Figure K-1. The interpolation approach consisted of the following steps:

1. **Select Chemicals of Concern**. Polychlorinated biphenyls (PCBs) were selected as the primary contaminant of concern (COC) for detailed data interpolation, because they delineate the vast majority of the contamination in the upper reach (approximately 85% of the RAL exceedance areas are driven by PCB exceedances) and have therefore been a primary focus of Pre-Design Investigation (PDI) sampling and analysis. Other COCs were also extensively sampled and analyzed throughout the upper reach, resulting in some localized areas where other COCs had RAL exceedances and PCBs did not. Other COCs with RAL exceedances were addressed separately from PCBs using a simpler interpolation method due to their more localized areas of concern. The interpolation results for all COCs were overlain on the PCB interpolation to develop the final combined RAL exceedance area footprint.

2. **Define Sediment Depths to be Used in Interpolation**. Interpolations were performed on two sediment depth-defined datasets that are applicable to RALs: surface sediment, defined as 0 to 10 cm; and subsurface sediment, defined as 0 to 45 cm (intertidal areas), 0 to 60 cm (subtidal areas), and shoaling intervals in the Federal Navigation Channel (FNC).

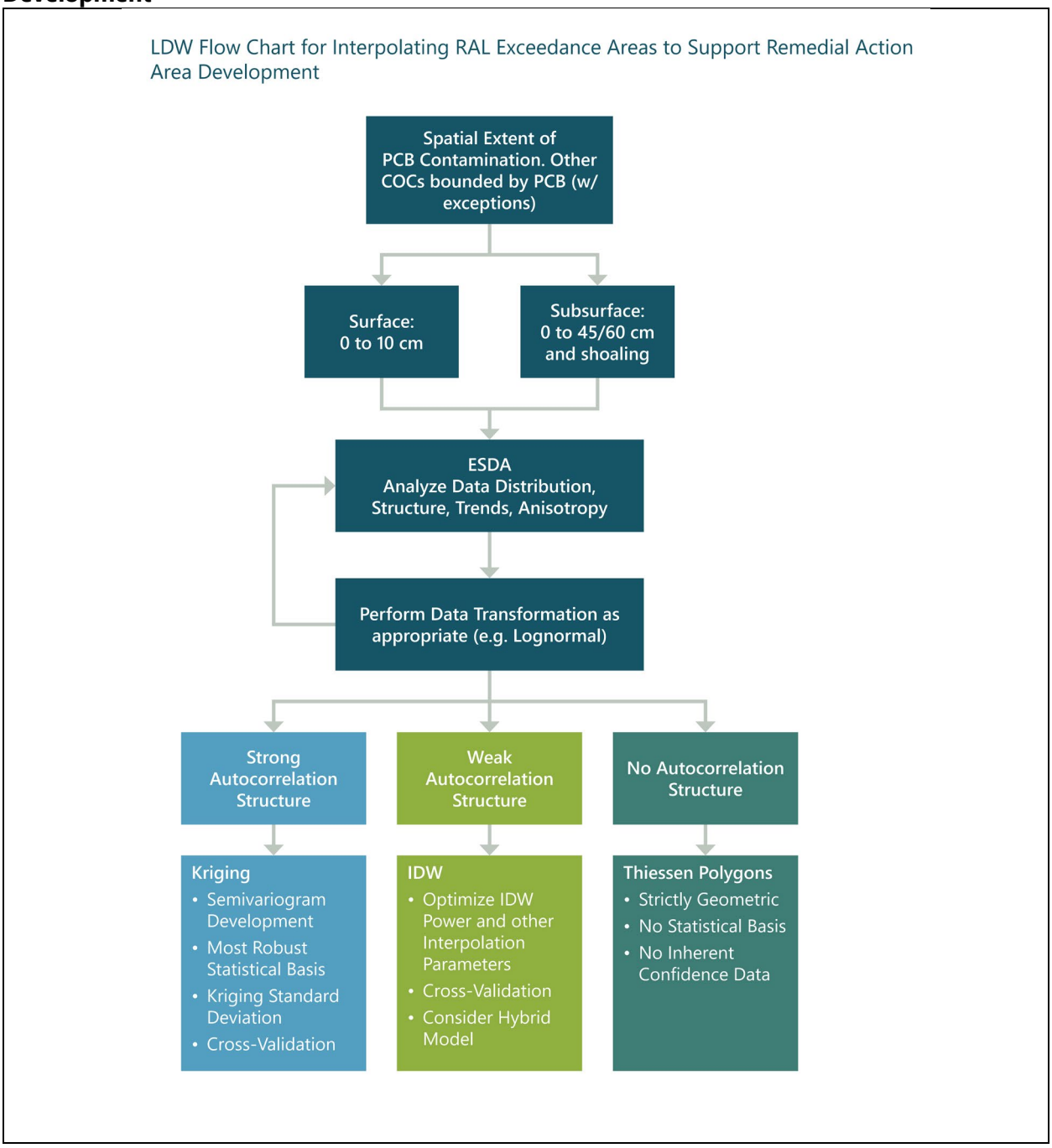
3. **Conduct Exploratory Spatial Data Analysis (ESDA)**. ESDA was performed on the PCB dataset to assess the statistical distributions of the PCB data and the characteristics of the

spatial distributions, including correlation structures, trends, and anisotropy (i.e., potential alignment of contaminated sediments with flow direction). The ESDA included preparation of sample point concentration maps, data histograms and probability plots, local variance maps, and preliminary semivariograms. Part of this analysis included determining whether data transformation (specifically, log transformation) was needed to address the skewness of the data prior to interpolation. ESDA results helped to inform the interpolation method selection for PCBs, as described in Step 4. Conducting ESDA on other COC data was not determined to be practical in discussion with the EPA interpolation technical team.

4. **Select Interpolation Method**. The inverse distance weighting (IDW) interpolation method had been used to define preliminary RAL exceedance area boundaries for PCBs in the LDW Feasibility Study and the Addendum to the PDI QAPP for Phase II (Phase II QAPP Addendum) (Anchor QEA and Windward 2021). Selecting the interpolation method to be used for RD required analyzing the full design dataset and conducting ESDA on the PCB data to select the most appropriate method(s). Three interpolation methods were considered for PCB datasets: kriging, IDW, and Thiessen polygons. Two different kriging methods were evaluated: ordinary kriging and indicator kriging. Based on ESDA results, kriging was found to be the preferred method for PCB interpolation because it provides the most robust information regarding spatial correlation structure and statistical confidence of the resultant predictions. Acceptable semivariogram models were developed for all areas and sediment depths in the upper reach to support kriging. Kriging was therefore selected for PCB interpolations and IDW was not considered further. Because areas with other COC RAL exceedances are small and localized, the RAL exceedance area boundaries for COCs other than PCBs were established using Thiessen polygons. See Section 2.4 for further discussion of interpolation method selection.

The initial work to develop the interpolation approach is described in greater detail in Sections 1.1 through 1.4 of this appendix. A detailed description of the ESDA and interpolation method selection is presented in Section 2. Indicator kriging input parameters are presented in Section 3, interpolation results are presented in Section 4, and interpolation uncertainty is discussed and quantified in Section 5.

**Figure K-1**
**Flow Chart for Interpolating RAL Exceedance Areas to Support LDW Remedial Action Area Development**




## 1.1 Chemicals of Concern

PCBs are the primary COC in the upper reach because PCB exceedances delineate the vast majority of contamination in the upper reach, encompassing approximately 85% of the RAL exceedance area.

Therefore, PCBs were the primary focus of the spatial interpolation efforts, including ESDA, semivariogram development, indicator kriging, and uncertainty analysis.

In localized areas, the PCB RAL exceedance area boundary was expanded using Thiessen polygons. Other COCs that locally determine the RAL exceedance area boundary include metals, polycyclic aromatic hydrocarbons (PAHs), other semivolatile organic compounds (butyl benzyl phthalate, benzoic acid, 4-methylphenol, phenol), and dioxins/furans, depending on the area.

## 1.2 Surface and Subsurface PCB Datasets

Interpolation was performed separately on surface PCB data (0 to 10 cm) and subsurface PCB data (0 to 45 cm, 0 to 60 cm, and shoaling intervals in FNC). Ultimately, these two datasets were combined to develop an integrated RAL exceedance area boundary that circumscribes both surface and subsurface PCB RAL exceedances.

**Surface Dataset**. Surface sediment PCB data were compared to a PCB RAL = 12 mg/kg-organic carbon (OC) (expressed on a carbon-normalized basis). There are 759 data points and 67 RAL exceedances (8.8% exceedance frequency) in the surface sediment PCB dataset.

**Subsurface Dataset**. The subsurface sediment PCB dataset was divided into different areas with three different RALs: 12, 65, and 195 mg/kg-OC, depending upon the sediment bed elevation, recovery category area, and whether the data were from shoaling areas in the FNC. There are 167 data points and 41 RAL exceedances (24.6% exceedance frequency) in the subsurface PCB dataset in RAL = 12 mg/kg OC areas. There are 123 data points and 16 RAL exceedances (13% exceedance frequency) in the subsurface PCB dataset in RAL = 65 mg/kg OC areas.[1] There are no exceedances in RAL = 195 mg/kg OC areas.[2]

For other COCs, surface and subsurface datasets were also used to interpolate RAL exceedance boundaries (using Thiessen polygons) and then combined to interpolate the data.

## 1.3 Organic Carbon Normalization of PCB Data

Consistent with the LDW Record of Decision (ROD), the PCB data were normalized to OC content for comparison to PCB RALs. A small percentage (approximately 10%) of data did not fall within the acceptable total organic carbon (TOC) range for OC normalization;[3] in those cases, RAL comparisons were made on a dry weight basis.

[1] Sample counts and exceedance statistics are presented on a location-specific basis. Note that some shoal areas are composed of multiple sample intervals/results, but only the maximum concentration was used to determine whether or not an exceedance is present at each particular shoal location.

[2] The 0–60 cm RAL of 195 mg/kg-OC PCBs applies to Recovery Category 2 and 3 subtidal areas with elevations above -18 ft mean lower low water in this reach of the LDW (see ROD Table 28).

[3] The acceptable OC normalization range is TOC ≥ 0.5% and ≤ 3.5%.

Mixed units, such as mixed OC-normalized and dry weight units, can be a confounding factor when interpolations are performed using ordinary kriging of PCB concentrations. However, mixed units are readily accommodated using indicator kriging methods (i.e., kriging of exceedance probability), as discussed in Section 2.

## 1.4 Upper Reach Segmentation

Interpolation methods were developed for the entire upper reach of the LDW. However, in some cases, interpolations could be improved by focusing on specific upper reach segments that exhibit similar hydrodynamic and sedimentary processes. In addition to the full upper reach, the following segments were evaluated during method development:

- **Lower Segment:** River mile (RM) 3.00 to RM 3.58, with a channel alignment of 312 degrees
- **Middle Segment:** RM 3.58 to RM 4.61, with a channel alignment of 348 degrees
- **Slip 6:** RM 4.18 to RM 4.27, an off-channel slip approximately perpendicular to the main channel
- **Upper Turning Basin:** RM 4.61 to RM 4.80
- **Norfolk Area:** RM 4.80 to RM 5.00, with the primary distribution of contamination along the east bank.

The upper reach segments are shown in Maps K-1a, K-1b, and K-1c. The average channel alignments are expressed as compass directions relative to 0 degrees true north. If interpolations could be improved on a segment-specific basis by refining the correlation structure or increasing the correlation distance of the semivariograms, the segment-specific semivariogram model replaced the full-reach model in those cases.

# 2 Exploratory Spatial Data Analysis

ESDA was performed on the PCB datasets to define the statistical and spatial characteristics of the data distributions and to help determine the most appropriate interpolation method. ESDA included preparation of sample point concentration maps to display raw, uninterpolated concentration distributions, analysis of statistical data distributions, local variance maps, and preliminary semivariograms. The results of the ESDA were used to select the interpolation method for the PCB data in collaboration with the EPA technical team. The interpolation work group determined that it was not practicable to perform a detailed ESDA for others COCs that affected only limited and localized areas.

## 2.1 Sample Point Concentration Maps

Sample point concentration maps are presented in Maps K-1a, K-1b, and K-1c for surface and subsurface datasets. These maps show the distributions of sample locations and concentrations, as

reported in the main text of this PDI Data Evaluation Report, without any interpolation or interpretation.

To prepare these maps, OC-normalized data and dry weight data that fell outside the acceptable range for carbon normalization had to be merged and expressed on a consistent basis. This was done by calculating the RAL exceedance ratios for any dry weight sample results and converting those results to an OC-normalized concentration with an equivalent RAL exceedance ratio. See Section 2.4 for further discussion of the treatment of mixed concentration units.

## 2.2 Statistical Distributions

Statistical distribution plots (histograms and probability plots) are presented in Attachment K-1. Separate plots are presented for surface and subsurface PCB datasets.

Both surface and subsurface PCB datasets are highly positively skewed, which is not unusual for environmental concentration data. Surface PCB data range over approximately seven orders of magnitude, from 0.0007 to 10,600 mg/kg OC. Subsurface PCB data range over approximately five orders of magnitude, from 0.008 to 950 mg/kg OC.

Log transformation of both surface and subsurface PCB data brings both datasets into reasonable conformance with a normal distribution (i.e., data are lognormally distributed). As a result, any interpolations performed using concentration data should be log-transformed to satisfy any underlying assumptions of normality, especially for ordinary kriging methods.

The log-transformed distributions exhibit a mild negative skewness. The left-hand tails of the log-transformed distributions are affected by a wide range of detection limits spanning multiple orders of magnitude. This is a result of combining datasets from multiple investigations and laboratories spanning nearly three decades, from 1995 to 2021.

## 2.3 Local Standard Deviation Maps

Local standard deviation maps for surface and subsurface datasets are presented in Maps K-2a and K-2b using Thiessen polygons. The local standard deviation is calculated for each polygon based on the differences in PCB concentrations between the sample in the central polygon versus the samples in all of its neighboring polygons.

These maps help identify areas where concentrations change quickly over short distances; interpolations may have a higher degree of uncertainty in such areas. However, many areas exhibiting a high degree of local deviation or variance (i.e., the square of the standard deviation) are in areas with concentrations below the RAL, where such variance would not likely result in exceedances. The deviations/variances in these areas are sometimes confounded by a high

percentage of undetected values, often with variable detection limits and analytical sensitivities, as indicated by the negatively skewed distributions in log space (see Section 2.2).

## 2.4 PCB Dataset Interpolation Method Selection

PCB dataset interpolation method selection was informed by the ESDA. Three interpolation methods (kriging, IDW, and Thiessen polygons) were evaluated for delineating the RAL exceedance area boundaries in the upper reach, as described in Section 1, Steps 1 through 4, and Figure K-1. Two types of kriging methods were evaluated: ordinary kriging and indicator kriging. The spatial correlation structures of the data were sufficiently well characterized to support the use of kriging for delineating PCB RAL exceedance areas in all segments and sediment depths in the upper reach. In general, kriging is a preferable interpolation method to IDW because kriging requires a more rigorous analysis of the spatial correlation structure of the data and more quantitative data regarding prediction uncertainty (Isaaks and Srivastava 1989).

Ordinary kriging directly interpolates PCB concentrations and generates a PCB concentration distribution map. Because of the skewness of the upper reach PCB data distribution (see Section 2.2), ordinary kriging was performed using the logarithms of the concentration data to conform to the underlying normality assumptions of the method (i.e., upper reach PCB data were lognormally distributed). Indicator kriging is probability kriging, and in this case, the indicator is the probability of exceeding the RALs. Samples that exceed the RALs are assigned a probability value of 1 (100%), and samples below the RALs are assigned a probability value of 0 (0%). Indicator kriging then interpolates the field of samples represented by zeroes and ones. Between sample locations, the indicator is a continuous variable spanning a range of probability values between 0 and 1 (0% to 100%).

During ESDA, semivariogram models were developed for both ordinary kriging, based on PCB concentrations (carbon-normalized or equivalent dry weight concentrations), and indicator kriging based on exceedance probabilities. The LDWG/EPA interpolation work group selected indicator kriging as the preferred interpolation method for the following reasons:

- Indicator kriging provides quantitative estimates of the statistical confidence of the RAL exceedance area boundaries.
- Indicator kriging is a nonparametric method that does not require log transformation to control highly skewed concentration data, such as the upper reach PCB data, as would be required for ordinary kriging.
- Indicator kriging can readily accommodate mixed units, specifically, mixed OC-normalized and dry weight concentrations and RALs.[4] In ordinary kriging, dry weight-based exceedances

[4] In the LDW, there is a finite range (from 0.5% to 3.5% TOC) over which PCB data are evaluated on an OC-normalized basis; outside of this range, data are evaluated on a dry weight basis without OC normalization.

must be expressed on an equivalent OC-normalized concentration with the same exceedance ratio to bring the dataset into a consistent set of units. This necessity introduces potential discontinuities and uncertainty in the spatial correlation structure. In indicator kriging, an exceedance is an exceedance, regardless of its basis; therefore, unit conversion is not necessary and discontinuities in the spatial correlation structure are minimized.

- Indicator kriging has been successfully applied to support RD and remedial action on other large sediment sites, in particular, the Lower Fox River, Wisconsin, in EPA Region 5 (Anchor QEA and Tetra Tech 2016; Thornburg et al. 2005).

# 3 PCB Dataset Indicator Kriging Input Parameters

Interpolation methods use a local neighborhood of surrounding data points to estimate the values at all unsampled points in the map domain. Indicator kriging interpolation methods are specified by the following input parameters:

- **Semivariogram Correlation Structure**. Semivariograms define the spatial correlation structure of the PCB indicator data (i.e., the strength and distance over which site-specific, inter-sample correlations occur). Semivariograms are used to assign sample weighting factors during interpolation, such that samples located closer to the estimation point are more strongly correlated to the estimation point and receive higher weighting factors.

- **Search Parameters**. Search parameters define how many neighboring data points are used to calculate the interpolated value of each estimation point, and over what distances and directions neighboring data points are included.

These parameters, as well as the use of site-wide versus segment-specific semivariogram models, and the specification of corresponding site-wide versus segment-specific input parameters, are presented in this section. In addition, this section discusses the geographic information system (GIS) raster computations that were used to combine subsurface areas regulated using different RALs, and to merge surface and subsurface interpolation layers into a single layer showing the combined footprint that captures the extent of RAL exceedances in both layers.

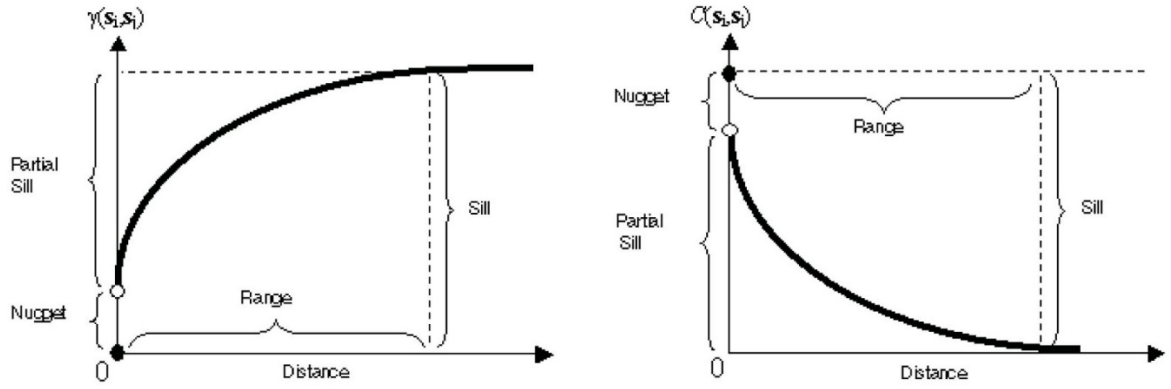
## 3.1 Semivariogram Correlation Structure

Semivariograms describe the site-specific spatial correlation structure of the data. For indicator kriging, the data are digital indicators (0 and 1) based on exceedance or non-exceedance of PCB RALs. Kriging uses the spatial correlation structure defined by the semivariograms to assign appropriate sample weighting factors during the interpolation process (Isaacs and Srivastava 1989).

A typical semivariogram structure, and its complementary function, the covariance structure, are shown in Figure K-2. Semivariance and covariance functions both measure the strength of statistical

correlation with distance. Semivariograms are developed by considering all possible combinations of sample pairs in the dataset and calculating the variance (i.e., differences between sample pairs) associated with increasing sample separation distances. Samples that are closer together are expected to be spatially correlated and therefore have a lower variance, or alternatively, a higher covariance, than samples spaced farther apart.

**Figure K-2**
**Typical Semivariogram Structure**




From: ESRI ArcGIS Pro 2.9, 2022.
https://pro.arcgis.com/en/pro-app/latest/help/analysis/geostatistical-analyst/semivariogram-and-covariance-functions.htm

The spatial correlation structure in semivariograms is described by the following three parameters:

- **Nugget**. The nugget is the y-intercept of the semivariogram and represents the inherent sample variance at any given location due to inherent field and laboratory variability and imprecision.
- **Range**. The range is the distance over which samples are spatially correlated. Within the range, the sample variance increases from a minimum value at the nugget to a maximum value at the sill.
- **Sill**. The sill is the variance at the end of the correlation range that represents the background population variance lacking any spatial correlation. The partial sill is the sill minus the nugget.

Semivariograms were developed separately for surface and subsurface PCB datasets, as described in Section 1.2. For the subsurface PCB dataset, semivariograms were developed separately for areas where RAL = 12 and RAL = 65 mg/kg OC are applicable. Semivariograms were developed on a site-wide basis (i.e., the entire upper reach) for both surface and subsurface datasets, but if interpolations could be improved on a segment-specific basis, they superseded the site-wide semivariogram model (see Section 1.4) for that segment. Upper reach segments are shown in Maps K-1a, K-1b, and K-1c.

The primary improvement that resulted in the use of some segment-specific semivariogram models was a longer correlation range, which provides a greater distance over which neighboring samples can be used for interpolation, and generally increases the accuracy of the interpolation. Site-wide

semivariogram models were superseded by segment-specific models in the middle segment of the surface dataset and in the middle and lower segments of the subsurface dataset.

Indicator kriging semivariogram spatial correlation plots and semivariogram models are compiled in Attachment K-2. Table K-1 shows the methods that were applied to each of the upper reach segments.

**Table K-1**
**Upper Reach Interpolation Methods**

| Upper Reach Area | | Indicator Kriging: Site-Wide | Indicator Kriging: Segment-Specific | Thiessen Polygons |
|---|---|---|---|---|
| ***Surface Sediment*** | | | | |
| **PCBs** | Lower segment (RM 3.00–RM 3.58) | X | | |
| | Middle segment (RM 3.58–RM 4.61) | | X | |
| | Slip 6 (RM 4.18–RM 4.27) | No Exceedances | | |
| | Turning Basin area (RM 44.61–RM 4.80) | X | | |
| | Norfolk area (RM 4.80–RM 5.00) | X | | |
| **Other COCs – All Areas** | | | | X |
| ***Subsurface Sediment*** | | | | |
| **PCBs** | Lower segment (RM 3.00–RM 3.58) | | X | |
| | Middle segment (RM 3.58–RM 4.61) | | X | |
| | Slip 6 (RM 4.18–RM 4.27) | X | | |
| | Turning Basin area (RM 4.61–RM 4.80) | X | | |
| | Norfolk area (RM 4.80–RM 5.00) | No Exceedances | | |
| **Other COCs – All Areas** | | | | X |

Notes:
COC: contaminant of concern
PCB: polychlorinated biphenyl
RM: river mile

Semivariogram model parameters (nugget, range, and sill) are summarized in Table K-2. Spherical semivariogram models provided a reasonable fit to the spatial correlation structures and were applied to all datasets for consistency. Isotropic models were used because no clear evidence of anisotropy could be discerned from the spatial correlation structures (i.e., insufficient evidence that contaminated sediment deposits were elongated with the flow direction of the waterway). The nugget variance was relatively well controlled at 17 to 25% of the sill value. The correlation range of the subsurface data (50 to 75 ft) was slightly longer than the correlation range of the surface data (30 to 45 ft), possibly because of the greater thickness of subsurface samples, which represents a longer time interval and longer averaging period compared to surface samples.

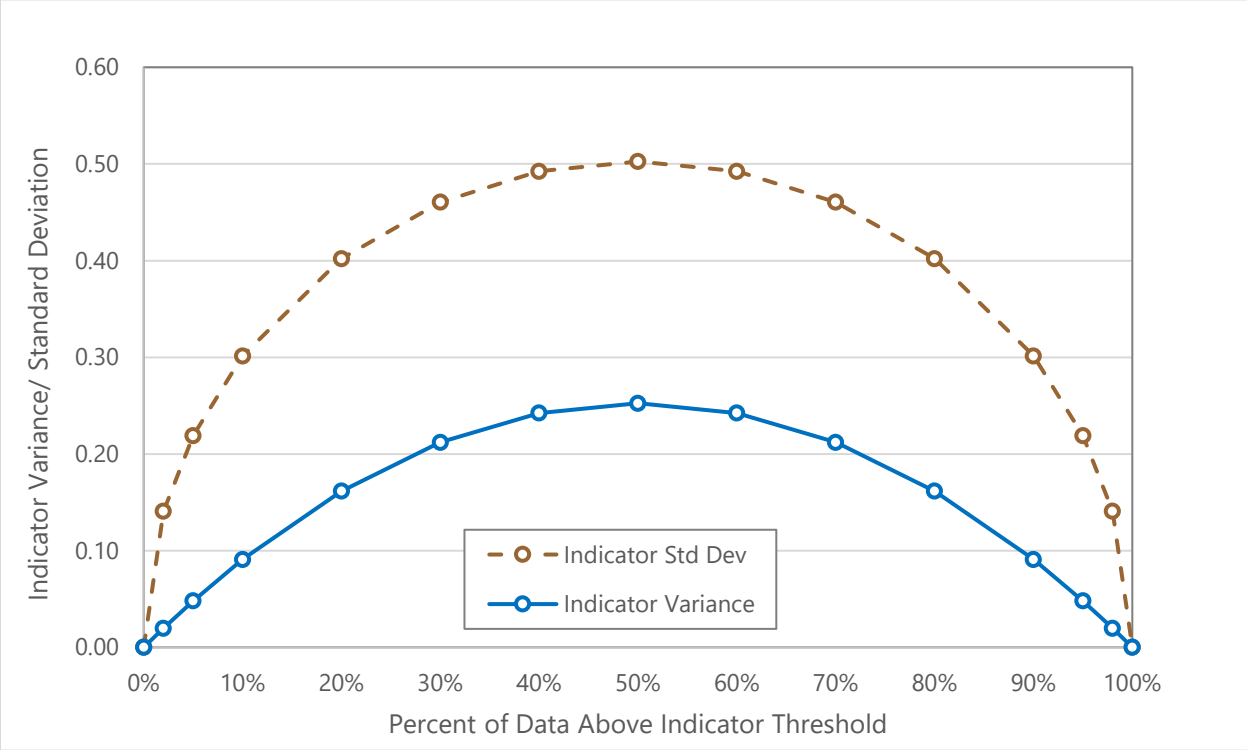
**Table K-2**
**Indicator Semivariogram Model Parameters**

| Depth | Surface | | Subsurface | | | | | |
|---|---|---|---|---|---|---|---|---|
| Indicator Threshold (mg/kg-OC) | 12 | | 12 | 65 | 12 | 65 | 12 | 65 |
| Segment | Full Reach | Middle | Full Reach | | Lower | | Middle | |
| ***Indicator Statistics*** | | | | | | | | |
| Indicator count | 759 | 405 | 331 | 331 | 112 | 112 | 177 | 177 |
| Indicator variance | 0.080 | 0.091 | 0.219 | 0.057 | 0.246 | n/a | 0.209 | 0.083 |
| ***Semivariogram Parameters*** | | | | | | | | |
| Variogram model | Spherical - Isotropic | | | | | | | |
| Range | 30 | 45 | 50 | 50 | 70 | No Exceedance | 75 | 75 |
| Nugget | 0.020 | 0.020 | 0.060 | 0.020 | 0.050 | | 0.040 | 0.020 |
| Partial sill | 0.095 | 0.090 | 0.178 | 0.065 | 0.210 | | 0.196 | 0.100 |
| Full sill | 0.115 | 0.110 | 0.238 | 0.085 | 0.260 | | 0.236 | 0.120 |
| Nugget (% sill) | 17% | 18% | 25% | 24% | 19% | | 17% | 17% |

Notes:
OC: organic carbon
PCB: polychlorinated biphenyl
RAL: remedial action level
ROD: Record of Decision

The sill value is an estimate of the population variance of the indicators. As shown in Figure K-3, the variance of the indicators depends on the percent of the data that exceeds the indicator threshold (i.e., the proportions of ones and zeroes in the indicator dataset). An exceedance frequency of 50%, wherein one-half of the data fall above and below the indicator threshold value, respectively, results in the highest theoretical variance, at 0.25. There is a greater percentage of data that exceeds an indicator threshold of 12 mg/kg OC in the subsurface dataset than in the surface dataset, and there is a greater percentage of data that exceeds an indicator threshold of 12 mg/kg OC in the subsurface dataset than that exceed an indicator threshold of 65 mg/kg OC. As a result, subsurface indicators based on a threshold of 12 mg/kg OC have the highest variances and semivariogram sill values, in the range of 0.24 to 0.26. Surface indicators and subsurface indicators based on a threshold of 65 mg/kg OC have lower variances and semivariogram sill values, in the range of 0.09 to 0.12.

**Figure K-3**
**Indicator Variance and Standard Deviation as a Function of Threshold Exceedance Frequency**




## 3.2 Search Parameters

Interpolation search parameters define how many neighboring data points are used to calculate the interpolated value of each estimation point, and over what distances and directions neighboring data points are included. For this work, quadrant searches were performed with the search axis oriented along the upper reach channel alignments, as listed in Section 1.4. A minimum of two samples and a maximum of five samples from each quadrant were used to perform the interpolations. The search radius was set to a value greater than the correlation range, typically two to three times the correlation range.

## 3.3 Indicator Kriging Raster Computations

Indicator kriging was performed using the Esri ArcGIS program (ArcGIS Desktop 10.8.1 and Geostatistical Analyst 10.8.1 extension, plus the Spatial Analyst 10.8.1 extension for raster analysis and manipulation). The geostatistical surfaces were exported to raster datasets with a raster cell size of 2 ft, which is an appropriate resolution on which to base RD. The PCB surface dataset was compared to a single RAL (RAL = 12 mg/kg OC), but in the subsurface dataset, different RALs applied in different areas. Therefore, indicator kriging was performed twice in the PCB subsurface dataset for

each of the two RALs: RAL = 12 and RAL = 65 mg/kg OC. The entire dataset was used for both of these subsurface interpolations to provide optimal boundary control; then, the two subsurface layers were cropped to their applicable RAL areas and spliced. If segment-specific interpolations were performed, their results replaced the values of the full-reach interpolation in the corresponding surface or subsurface rasters, as applicable.

Using a GIS raster calculation, the surface and subsurface interpolation layers were combined into a single layer showing the PCB RAL exceedance footprint of both layers. All interpolation layers used the same grid and were registered to the same origin, thereby streamlining raster computations. Each grid cell in each interpolation layer has an interpolated indicator value, a continuous variable between zero and one. ArcGIS software stacks the two rasters, selects the highest indicator value in each grid cell, and exports that value to a new layer, which represents the combined exceedance probability for both surface and subsurface datasets.

# 4 Interpolation Results

RAL exceedance area maps are presented in the K-3 and K-4 map series. The K-4 map series will provide the foundation for RD and will be the starting point to overlay engineering and constructability considerations, which will extend the horizontal boundary for remedial action in many locations.

Three PCB interpolation maps are presented: surface sediment, subsurface sediment, and combined surface and subsurface sediment, which represents the combined horizontal extent of interpolated PCB contamination from both layers (Maps K-3a, K-3b, and K-3c). The 50% probability contour represents the median, central tendency, and best estimate of the horizontal RAL exceedance boundary (Anchor QEA and Tetra Tech 2016; Thornburg et al. 2005). Other contours including the 20%, 30%, 40%, 50% (median), 60%, 70%, and 80% probabilities of exceedance are provided for comparison in Maps K-3a, K-3b, and K-3c. The indicator kriging contours represent the probabilities of exceeding the applicable RALs, expressed in units of percent. The more extreme 10% and 90% probabilities of exceedance are not presented because they are within the inherent error of the analysis and are more prone to interpolation artifacts. A second set of maps shows the median PCB RAL exceedance area boundary overlain with Thiessen polygons for COCs other than PCBs that extend beyond the median PCB boundary (Maps K-4a, K-4b, K-4c, and K-4d). Like the PCB interpolations, the Thiessen polygons include the combined horizontal extent of contamination from other COCs in both surface and subsurface intervals. Other COCs that extend the RAL exceedance boundaries include metals, PAHs, other semivolatile organic compounds (butyl benzyl phthalate, benzoic acid, 4-methylphenol, phenol), and dioxins/furans, depending on the area. This analysis used the RALs from Table 28 in the ROD (EPA 2014) and the RALs for carcinogenic polycyclic aromatic hydrocarbons (cPAHs) in the 2021 Explanation of Significant Differences (EPA 2021). Overlaying the

interpolated exceedance areas for PCBs with Thiessen polygons for other COCs captures all areas with likely COC exceedances. Boeing Plant 2 early action area (EAA), T-117 EAA, and the Jorgensen Forge EAA are excluded from the RAL exceedance areas because these areas have been remediated and are being monitored. The Norfolk EAA was remediated in 1999, more than 10 years earlier than the other EAAs. PDI data have been collected within the Norfolk EAA to bound RAL exceedances along the shoreline. Thus, the PDI data collected within the Norfolk EAA were included in the interpolation on Map K-4d.

The intertidal plot for the enhanced natural recovery/activated carbon (ENR/AC) pilot study is also located within the upper reach. For the pilot study, an ENR layer was placed at RM 3.9E in 2017: one subplot with ENR alone and one subplot with ENR mixed with AC. The ENR material was a mixture of clean sand and gravel and was analyzed for all the RAL chemicals prior to construction to ensure that the ENR material concentrations were below LDW cleanup levels (Amec Foster Wheeler et al. 2018). ENR material was placed in both subplots at an average thickness of approximately 25 cm. The surface sediment within the ENR/AC pilot study area is physically distinct from the surrounding surface sediment. The PCB concentrations in the ENR material sampled at five locations during the PDI Phase II sampling ranged from 1.82 to 17.5 µg/kg. Because the surface sediment on the ENR/AC intertidal plot has been monitored and PCBs concentrations are well below RALs, PCB interpolations were not extended into the ENR/AC pilot study intertidal plot (Map K-3a). In addition, Thiessen polygons associated with butyl benzyl phthalate concentrations exceeding the RAL at locations R31 and AN-47 were not extended into the pilot plot, because this compound was not detected in the ENR material.

The 0–45-cm subsurface sediment interval within the intertidal ENR/AC pilot plot includes both ENR material and underlying sediment. Several subsurface intervals from five locations within the plots were analyzed for PCBs and arsenic as part of the PDI. PCB and arsenic concentrations were below the RALs in the 0–45-cm interval below the current mudline and in the 0–45-cm interval below the ENR placement. The PDI locations were selected to characterize the areas with the greatest surface sediment PCB concentrations prior to ENR placement.

Two intertidal subsurface samples (IT622 and IT257) adjacent to the ENR/AC pilot plot had dioxin/furan toxic equivalents (TEQs) greater than the RAL of 28 ng/kg (Map 3-4e). The ENR material had a dioxin/furan TEQ of 2 ng/kg prior to construction. Based on an average depth of 25 cm of ENR material, the potential for a 0–45-cm RAL exceedance in the ENR/AC plot was assessed. In order for the 0–45-cm interval to exceed the RAL, the dioxin/furan TEQ in the 20-cm interval of sediment below the ENR layer would need to be 62 ng/kg. The greatest dioxin/furan TEQ reported for the three surface sediment samples within the ENR/AC pilot plot prior to construction was 33.7 ng/kg (IT257). The greatest dioxin/furan TEQ in the subsurface intervals adjacent to the ENR/AC pilot plots

was 31.8 ng/kg (IT622). Therefore, the dioxin/furan Thiessen polygons associated with IT627 and IT257 were not extended into the ENR/AC plot.

Based on PDI sampling, 0–45-cm PCB RAL exceedances were reported for two locations adjacent to the southern ENR/AC pilot subplot (IT627, IT257) (Map 3-4e). In order to determine if the PCB subsurface interpolations should extend into the ENR/AC plot, existing data were reviewed to assess the potential for 0–45-cm RAL exceedances of PCBs following ENR placement.

The ENR material in the southern subplot had PCB concentrations ranging from 3.96 to 7.55 µg/kg and TOC ranging from 0.06% to 0.15% in the five PDI samples. For a 0–45-cm PCB RAL exceedance, the sediment below the ENR layer would need to have a PCB concentration of 3,300 µg/kg with a TOC of 2% to exceed the RAL. Nine surface sediment samples collected within the subplot had a maximum PCB concentration of 1,060 µg/kg. There were three cores collected in the subplot, with a maximum PCB concentration of 3,000 µg/kg in the 0–1-ft interval. The PCB concentrations in the adjacent 0–45-cm samples were 1,210 µg/kg (IT627) and 3,380 µg/kg (IT257). Based on this analysis, the subsurface PCB interpolation was not extended into the southern subplot. The uncertainty regarding the subsurface PCB concentrations in this area will be evaluated in 30% design to determine if additional characterization is warranted as part of the Phase III investigation.

# 5 PCB Uncertainty Analysis

The confidence or uncertainty of the PCB RAL exceedance area boundary was assessed using three independent lines of evidence:

- Indicator kriging probability contours
- Cross validation prediction errors
- Kriging standard errors (KSEs)

The uncertainty of RAL exceedance area boundaries defined by Thiessen polygons for other COCs in small, localized areas will be evaluated on a location-specific basis during RD using best professional judgment in consideration of the magnitude of the exceedance.

## 5.1 Indicator Kriging Probability Contours

Indicator kriging probability contours are the primary line of evidence for assessing the uncertainty of the PCB RAL exceedance area boundary. The indicator kriging method was selected, in part, because it has the distinct advantage of providing quantitative, probabilistic information directly in the kriging output data. In addition, the probability contours can be used throughout the RD process to continually assess the confidence of the proposed remedy.

The boundary corresponding to the 50% probability of exceedance is assumed to be the initial basis for RD. During the design process, the remediation footprint will generally be expanded beyond the

RAL exceedance boundary as a result of: a) simplifying the curved and irregular RAL exceedance area boundaries to more rectilinear but fully encompassing boundaries to provide a more constructible design, and b) in dredging areas, extending the side slopes of the dredge prism beyond the minimum required dredge boundary. During 30% design, locations with greater uncertainty may be addressed through the engineering of the cleanup footprint and/or by identifying the need for additional (Phase III) data to reduce uncertainties. For these reasons, a higher level of confidence will generally be achieved during the design process.

Where indicator probability contours are tightly compressed, there is more certainty in the location of the RAL exceedance area boundary. Where the probability contours diverge and separate, there is more uncertainty in the RAL exceedance area boundary. In general, areas of diverging probability contours in critical remediation areas can be addressed by collecting Phase III PDI samples to help reduce the uncertainty in those areas, or by designing remedial action area boundaries to encompass such areas of greater uncertainty.

## 5.2 Cross-validation Statistics

Cross-validation (also called "drop one" cross validation) prediction error statistics were calculated in ArcGIS Geostatistical Analyst as a secondary line of evidence to assess interpolation uncertainty. Cross-validation provides an estimate of interpolation prediction error at each individual sample location. First, the sample result in question is removed from the dataset; then, the kriging algorithm predicts (i.e., interpolates) the value at the missing sample location using only the surrounding data. This procedure is repeated for every sample location. Then, observed and predicted indicators are compared and prediction error statistics are compiled across the entire dataset. Cross-validation prediction error statistics for surface and subsurface kriging applications, in both RAL = 12 and RAL = 65 mg/kg OC areas, are shown in Table K-3.

**Table K-3**
**Cross-Validation Prediction Error Statistics**

| Depth | Surface | | Subsurface | | | | |
|---|---|---|---|---|---|---|---|
| Indicator Threshold (mg/kg-OC) | 12 | 12 | 12 | 65 | 12 | 12 | 65 |
| Segment | Full Reach | Middle | Full Reach | Full Reach | Lower | Middle | Middle |
| ***Prediction Error Statistics*** | | | | | | | |
| Count | 759 | 405 | 331 | 331 | 112 | 177 | 177 |
| Mean | 0.003 | 0.002 | -0.007 | -0.0003 | -0.014 | -0.001 | -0.001 |
| RMSE | 0.241 | 0.255 | 0.432 | 0.225 | 0.489 | 0.408 | 0.265 |
| Max KSE[1] | 0.355 | 0.339 | 0.516 | 0.308 | 0.535 | 0.504 | 0.359 |

Notes:
1. Calculated as the square root of full sill value in the semivariogram model; see Table K-2.

KSE: kriging standard error
OC: organic carbon
RMSE: root mean squared error

The mean prediction error for the various indicator kriging applications ranges from -0.014 to +0.002 (-1.4 to +0.2%). These values are very close to zero and therefore show a minimal amount of bias in the overall predictions.

The root mean squared error (RMSE) ranges from 0.24 to 0.26 (24 to 26%) in the surface kriging predictions and 0.23 to 0.49 (23 to 49%) in the subsurface kriging predictions. Higher RMSE values are associated with subsurface indicator kriging applications using a threshold value of 12 mg/kg OC, because a greater percentage of these data exceed the indicator threshold value, resulting in higher variances and semivariogram sill values (see Table K-2).

It should be noted that cross-validation prediction errors are derived by removing known sample data from the specific points that are being estimated, thus effectively doubling the inter-sample separation distance at the point of interest. As a result, cross-validation prediction error statistics are likely overestimated.

## 5.3 Kriging Standard Error

Kriging standard error (KSE) results are shown on Map K-5. KSE data are considered the lowest priority line of evidence in this uncertainty analysis, because they are solely a function of the sample distributions and the assigned semivariogram models, and they do not consider the local variance of the actual data.

The maximum KSE is estimated from the full sill value of the semivariogram models, as compiled in Table K-3. The full sill value is an estimate of the indicator population variance, and the square root of the sill value is an estimate of the maximum KSE value that would apply in areas with no neighboring data within the inter-sample correlation distance (i.e., within the range, Table K-2). More densely sampled areas with smaller inter-sample spacings within the range of spatial correlation have lower KSE value.

The maximum KSE ranges from 0.34 to 0.36 (34% to 36%) in the surface kriging applications and 0.31 to 0.54 (31% to 54%) in the subsurface kriging applications. Kriging predictions in subsurface RAL = 12 mg/kg OC areas generally have higher KSE values, largely because of the greater percentage of data that exceeds the indicator threshold, and thus higher population variances for those datasets (see Table K-2).

In all cases, the cross-validation RMSE is less than the maximum KSE. The RMSE averages about 80% of the maximum KSE. This indicates that inter-sample correlations are helping to improve the indicator kriging predictions and that the effective KSEs are lower than the maximum sill value.

The KSE maps in Map K-5 show that the KSE is largely a function of sample density and spacing, with lower KSE values in areas with high sample density and close inter-sample spacing. As expected, the more densely sampled areas also correspond to areas of greater concern for potential remediation, so the upper reach sampling design has effectively reduced the KSE where it matters most. The KSE maps are also sensitive to the semivariogram sill values, resulting in some KSE discontinuities at segment boundaries where two interpolation maps with different population variances are spliced.

# 6 References

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# 7 Attachments

Attachment K-1 PCB Statistical Distributions

Attachment K-2 PCB Semivariograms